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S.Frauendorf

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A SYSTEMATIC INVESTIGATION OF THE CORIOLIS ANTIPAIRING EFFECT IN THE RARE EARTH REGION INCLUDING PROJECTION ONTO EXACT PARTICLE NUMBER AND ANGULAR MOMENTUM

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# A SYSTEMATIC INVESTIGATION OF THE CORIOLIS ANTIPAIRING EFFECT IN THE RARE EARTH REGION INCLUDING PROJECTION ONTO EXACT PARTICLE NUMBER AND ANGULAR MOMENTUM

Сбъслиношали пиститут :Deleobalie名 TEHA

#### Summary

The coriolis antipairing effect is investigated for the rare earth nuclei. For this a new two-parameter expression for the pairing strength is introduced which is adjusted to the even-odd mass-differences. Good agreement with the experimental results concerning the linear part of the moment of inertia as a function of the square of the angular velocity can be reached if projection onto exact particle number is taken into account. The latter causes an essential stabilizytion of the pair-correlations. The critical angular velocity for the transition from the superfluid to the normal state is defined and calculated. It is substantially increased by projection onto exact particle number whereas it remains almost unchanged by projection onto exact angular momentum. The critical angular velocity at which the neutron pairing vanishes is systematically larger than the angular velocity at which back-bending is observed. From this it is concluded that back-bending cannot be caused by a rapid transition from the suprafluid to the normal state.

### 1. Introduction

The first observation of the irregular spacing of the yrast-levels in even-even rare earth nuclei/1/ has stimulated a number of experimental and theoretical investigations of this interesting phenomenon called back-bending (bb). As discussed in the reviews/2-5/on the subject the most likely explanations for bb are:

- The rapid transition from the suprafluid to the normal state caused by the Coriolis Antipairing Effect /6/ (CAP).

- The decoupling of two neutrons from the rotating core and the alignment of their angular momenta with that of the core/7/ (Rotational Alignment Effect, RAL).

As shortly sketched in the following it is not yet clear which of the two effects is the dominating mechanism causing bb.

In refs.<sup>/8-10</sup>/the yrast-levels of <sup>162</sup>Er and <sup>166-170</sup>Yb are well reproduced by calculations based on the CAP. The authors consider their results as a strong evidence for the phase transition-picture. On the other hand, in refs.<sup>11,11</sup> a good description of the yrast-levels of all even-even rare earth nuclei is achieved with the help of a semiphenomenological particle-plusrotor model. However the model contains some parameters which are neither fixed by independent experiments nor calculated.

The experimentally observed pattern of occurence or missing of bb in adjacent odd mass and even-even nuclei can be understood in the framework of RAL. This fact is considered in refs.  $^{/5/}$  as a kind of experimental indication that bb is caused by RAL. However in ref. $^{/4/}$  it is argued that it is also possible to interpret the mentioned pattern in terms of CAP.

One can investigate the relative importance of CAP and RAL by means of models which take into account both effects. This is done in the investigations of few-level models iof refs. /12,13/ The authors find out that in most cases bb is due to the decoupling of two particles (RAL) but do not exclude a phase transition for some outsides  $^{/13/}$ . It is argued in ref. $^{/4/}$  that these models do not take into account the change of the moment of inertia of the core via the CAP and, therefore, disfavour the possibility of a transition to the nonsuprafluid state. In ref. /14/ the Hartree Fock-Bogoljubov approach is used. According to this calculation bb  $in^{162}$  Er is due to the decoupling of two neutrons.

In ref.<sup>/15/</sup> the transition from the supra fluid to the normal state is estimated to take place at a higher angular momentum than the decoupling of two neutrons (RAL). Consequently the RAL, which is estimated to appear just at the angular momentum where bb is observed, is supposed to cause bb. In ref.<sup>/16/</sup> the CAP as origin of bb in  $^{154}$ Gd is ruled out analysing the spectrum by means of a model of crossing bands.

In the present work a systematic analysis of CAP is carried out for the eveneven nuclei in the rare earth region. Comparing with previous investigations of CAP in refs. /16-22/ the influence of conservation of particle number and angular momentum is studied. By means of a systematic comparison with the experimental data on the spacing of the yrast levels it is investigated whether the calculations based on the CAP do reproduce bb in a quantitative way or whether there are significant deviations from the observed pattern. The results of this comparison are considered as an evidence in disfavour of the interpretation of bb in terms of CAP.

Although the present work mainly concerns the interpretation of bb it should be mentioned that the results are of more general interest. For an interpretation of nuclear structure at high angular momentum it is important to know at which angular frequency the transition from the suprafluid to the normal state takes place. The present work provides a new estimate of this quantity based on a particle number conserving description of the pair-correlations.

The expressions for the energy of the yrast are derived in sections 2 and 3. Section 4 is devoted to the choice of the deformed single particle potential and the determination of the pairing strength. The results of the calculations for the region of low angular momentum are discussed in section 5. In section 6 the critical frequency of the break-down of pairing is introduced. This definition turns out to be useful for the discussion of the transition from the suprafluid to the normal state at high angular momentum (section 7).

## 2. The Rotational Energy Calculated by Means of a Particle Number Conserving Description of Pairing (Q-Projection)

As usual in literature  $^{/17-23/}$  we define CAP as a uniform weakening of the pair-correlations in the rotating nucleus. The strength of pairing is fixed, like in ref.  $^{/22/}$ . by means of the gap-parameter  $\Lambda$  the value of which is obtained by minimizing the total energy  $E_1(\Delta)$  for a given angular momentum I. The expression for  $E_1(\Delta)$  is derived assuming that all nonadiabatic effects (but CAP) can be neglected. As regards the most important ones  $^{/22/}$ , the influence of rotation on the deformation of the nucleus is not expected to be very essential for the well deformed nuclei of rare earth region (see refs. (22,24) ) and the discussion of section 5). However, it is not clear from the beginning whether the influence of rotation on the single (-quasi-) particle degrees of freedom is important or not. Rather, this effect is excluded in order to investigate what follows from the assumption that only CAP is responsible for bb and whether these results are compatible with the experimental findings. This kind of indirect argument was chosen because it is relatively simple to carry out calcula-. tions taking into account only CAP whereas, the inclusion of the single-particle degrees of freedom demands a much larger computa-

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tional effort. Moreover, in section 7 it will be shown that a part of the results remains valud even in the case that the neglected RAL is expected to be significant.

As only the influence of rotation on the gap parameter  $\Delta$  is considered,  $E_I$  for a given value of  $\Delta$  corresponds to the energy of adiabatic rotation. Restricting to the ground state bands of even-even nuclei  $E_I$  reads

$$E_{1}(\Delta) = E_{0}(\Delta) + \frac{I^{2}}{2 f(\Delta)}, \quad \hat{I} = \sqrt{I(I+1)}, \quad (2.1)$$

The expressions for the ground state energy  $E_0$  and the moment of inertia 3 are calculated using BCS-functions projected onto particle number N ( $\emptyset$  -projection). It is assumed that the pair-correlations are sufficiently well described by the Hamiltonian of monopole pairing (see, e.g., ref.  $^{/25/}$ )

 $H = H_{sp} - GP^{+}P, \ H_{sp} = \sum_{i} \epsilon_{i} c_{i}^{+} c_{i}, \ P^{+} = \sum_{i>0} P_{i}^{+}, \ (2.2)$ 

where  $\epsilon_i$  is the energy of the single-particle level i in a deformed axialsymmetric shell model potential. The operator  $c_i^+$  generates one particle on the level i,  $p_i^+$ a pair on the time reversed states i,i, i.e.,  $P_i^+ = c_i^+ c_i^+$ . The symboli 0 means that the sum runs only over states with a positive projection of the angular momentum on the symmetry axis. In order to simplify the notation, the Hamiltonian and the derived expressions are only written for one kind of particles. The generalization in the case of protons and neutrons (in the following denoted by Z and N, respectively) is obvious. The ground state wave function is approximated by means of the BCS-vacuum denoted by  $|\Delta, \lambda\rangle$  from which the component with the exact particle number N is projected out, i.e.,

$$|\Delta, N\rangle = \Re_0^{-1/2} Q_N |\Delta\lambda\rangle, \quad \Re_0 = \langle \Delta, \lambda | Q_N | \Delta, \lambda\rangle. \quad (2.3)$$

The realization of the projection operator  $Q_N$  is described in the appendix. The BCS-function has the well known structure (see, e.g., ref.  $^{25/}$ )

$$|\Delta, \lambda \rangle = \prod_{i>} (u_i + v_i P_i^+) |0\rangle, \quad \frac{u_i^2}{v_i^2} = \frac{1}{2} (1 \pm \frac{\epsilon_i - \lambda}{\sqrt{(\epsilon_i - \lambda)^2 + \lambda^2}}).(2.4)$$

The chemical potential  $\lambda$  is fixed for a given value of  $\Delta$  by the condition

 $2\sum_{i>} v_{i}^{2}(\Delta) = N.$  (2.5)

The ground state energy as a function of  $\Delta$  is obtained as the expectation value of H with respect to the state  $|\Delta, N > :$ 

 $E_{0}(\Delta) = \langle \Delta, N | H_{sp} | \Delta, N \rangle - G \langle \Delta, N | P^{+}P | \Delta, N \rangle.$  (2.6)

The explicite expression is given in the appendix. The moment of inertia is obtained by means of the cranking model (see e.g. ref.  $^{25/}$ ). According to this model one calculates the energy of the system in a frame of reference rotating with the angular velocity  $\omega$  around the x-axis. The corresponding Hamiltonian has the form

 $H_{\omega} = H - \omega J_{x}, J_{x} = \sum_{ij} j_{ij}^{x} c_{i}^{+} c_{j}, \qquad (2.7)$ 

where  $j_{ij}^{x}$  denotes the matrix element of the x-component of the single-particle angular momentum operator. In order to obtain the adiabatic rotational energy as a function of  $\Delta$  the term  $\omega J_{x}$  is taken into account in second order perturbation theory starting from  $|\Delta, N>$ . The moment of inertia equals -2 times the coefficient of the term quadratic in  $\omega$ .

The operator  $J_{x}$  generates from  $|\Delta,N>$  only states of the type

 $|\Delta, N, ij\rangle = \mathfrak{N}_{ij}^{-\frac{1}{2}} c_i^+ c_j^+ Q_{N-2} |\Delta, \lambda, ij\rangle, \ \mathfrak{N}_{ij} = \langle \Delta, \lambda, ij | Q_{N-2} | \Delta, \lambda, ij\rangle, \ (2.8)$ 

where  $|\Delta, \lambda, i\rangle$  denotes the BCS-vacuum with levels i,j blocked. In the appendix is shown that II is diagonal within the orthonormal set  $\{|\Delta, N\rangle, |\Delta, N, ij\rangle\}$ . This is only true for the special set of "projected twoquasiparticle states" (2.8) generated by  $J_x$ .

The Hamiltonian is not diagonal for states of the type "two-quasiparticles on time reversed states". However, these states contribute only to higher orders of perturbation theory. By treating  $\Delta$  as a free parameter these contributions are taken into account in an average but nonperturbative way. The fact, that H is diagonal, is also connected with the choice of the simple pairing interaction between the particles. In the case of a more realistic interaction this property gets lost  $^{/26/}$ .

Using second order perturbation theory one obtains for the moment of inertia

 $\mathfrak{G}(\Delta) = 2\Sigma \frac{|\langle \Delta, N, ij| J_x | \Delta, N \rangle|^2}{E_{ij} - E_0}, E_{ij} = \langle \Delta, N, ij| H| \Delta, N, ij \rangle. \quad (2.9)$ 

The explicite expressions for  $E_{ij}$  and  $<\Delta,N,ij|J_x|\Delta,N>$  are given in the appendix. From the explicite form of the matrix-element follows

$$\mathcal{J}(\Delta) = 4 \sum_{i > j > \frac{(u_i v_j - u_j v_i)^2 (|j_{ij}|^2 + |j_{ij}|^2)}{E_{ij} - E_0} (\frac{\eta_{ij}}{\eta_0})^4 .(2.10)$$

The total ground state energy and the moment of inertia are the sums of the corresponding contributions from protons and neutrons. As is discussed in more detail in the appendix, the Q-projection operator is approximated by a sum of 8 terms. In order to find the minimum of the total energy with respect to the gap-parameters  $\Delta_Z$  and  $\Delta_N$  the expressions  $E_Z(\Lambda_Z)$ ,  $E_N(\Lambda_N)$ ,  $\oint_Z(\Lambda_Z)$  and  $\oint_N (\Delta_N)$  are calculated at 8 points of  $\Lambda_Z$  or  $\Delta_N$  within an interval from 0 to 1.8 MeV. The value of  $E_I(\Lambda_Z, \Lambda_N)$  between the meshpoints is obtained by interpolation with 4th order polynomials. This method turned out to be sufficiently accurate and fast.

#### 3. <u>Conservation of Angular Momentum</u> (P<sub>1</sub>-Projection)

In refs.<sup>(3,9)</sup> it is discussed that if the internal structure of the nucleus rapidly changes with uncreasing angular momentum the quasiclassical cranking model may become a bad approximation. One way to take the conservation of angular momentum into account is to project out the components with the angular momentum  $I(P_{\rm I}$ -projection) from the basic wave functions (2.3) and (2.8). In refs.<sup>(27, 28)</sup> it is shown an approximate evaluation of the projection operator  $P_I$  leads to the same expression for the rotational energy as obtained in the cranking model. Only the ground state energy  $E_0$  is renormalized:

$$E_{0} = E_{0} - \frac{\langle \Delta, N | J_{x}^{2} | \Delta, N \rangle}{g_{nx}}$$
 (3.1)

where the Peierls-Yoccoz moment of inertia  $J_{\rm PY}$  can be written in good approximation/29/as

$$\mathfrak{I}_{\mathbf{P}\mathbf{Y}} = \frac{\langle \Lambda, \mathbf{N} | \mathbf{J}_{\mathbf{x}} (\mathbf{H} - \mathbf{E}_{0}) \mathbf{J}_{\mathbf{x}} | \Lambda, \mathbf{N} \rangle}{2 \langle \Delta, \mathbf{N} | \mathbf{J}_{\mathbf{x}}^{2} | \Lambda, \mathbf{N} \rangle^{2}}.$$
(3.2)

Using the matrix-elements of the appendix one obtains

$$<\Delta, N | J_{x} \left( \frac{11 - E}{1} \right) J_{x} | \Delta, N > =$$
  
= 2 \Sigma (u\_{i}v\_{j} - u\_{j}v\_{i})^{2} (|j\_{ij}^{x}|^{2} + |j\_{ij}^{x}|^{2}) (\frac{F\_{ij} - E}{1} \right) (\frac{\eta\_{ij}}{\eta\_{0}})^{\frac{1}{2}} .

The expressions are to be understood as sums of the contributions from the protons and the neutrons. In refs.<sup>(30.31)</sup> is shown that a more accurate account of the conservation of angular momentum leads to corrections to the moment of inertia. However, the magnitude of those contributions seems to be not yet clear (compare refs.<sup>(27,31)</sup>). Thus, the cranking-expression for the moment of inertia has been kept unchanged.

An accurate evaluation of the  $P_I$ -operator leads also to corrections in the rotational energy depending on higher powers of the angular momentum than  $I^2$ . The relevance of these terms to the subject of this work should be investigated because they.

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are connected with restoring a violated symmetry. It is rather complicated to carry out the P<sub>I</sub> -projection within the whole basis (2.3), (2.8), but one can hope to estimate the corrections by means of the simple projection approach that neglects the admixture (2.8). The same method is used in ref.<sup>/8/</sup> For the evaluation of the overlap integrals an approximation proposed in ref.<sup>/32/</sup> is used. Then the energy equals

$$\begin{split} & \mathrm{E}_{\mathrm{I}} = \mathrm{E}_{0} + \frac{2 < \Delta, \mathrm{N} | \operatorname{J}_{x}^{2} | \Delta, \mathrm{N} >}{\int \int d\beta \sin^{3}\beta \, \operatorname{d}_{00}^{\mathrm{I}}(\beta) \, \exp\left(-\frac{1}{2} < \Delta, \mathrm{N} | \operatorname{J}_{x}^{2} | \Delta, \mathrm{N} > \sin^{2}\beta\right)}{\int \partial \beta \sin \beta \, \operatorname{d}_{00}(\beta) \, \exp\left(-\frac{1}{2} < \Delta, \mathrm{N} | \operatorname{J}_{x}^{2} | \Delta, \mathrm{N} > \sin^{2}\beta\right)}, \\ & \text{where } \operatorname{d}_{00}^{\mathrm{I}}(\beta) \text{ denotes the reduced Wigner } \operatorname{d}_{\mathrm{function.}} \mathrm{In \ second \ order \ of \ } 1 / < \Delta, \mathrm{N} | \operatorname{J}_{x}^{2} | \Delta, \mathrm{N} > \sin^{2}\beta)} \\ & \text{this expression becomes the renormalized} \\ & \text{ground \ state \ energy \ } (3.1) \ \text{and \ a \ rotational} \\ & \text{energy, \ } quadratic \ in \ \mathrm{I}, \ but \ with \ the \ moment} \\ & \text{of \ inertia \ } \operatorname{J}_{\mathrm{PY}} \ instead \ of \ \ensuremath{\mathcal{J}} \ . \ The \ occurrence} \\ & \text{of \ } fact \ that \ the \ contributions \ } (2.8) \ are \\ & \text{not \ taken \ into \ account.} \end{split}$$

## 4. Choice of Parameters

The basic input parameters needed for the calculations are the energies and matrix-elements  $j_{ij}^x$  in the deformed shell model potential and the strength of the pairing interaction. As deformed potential well the Nilsson-model in the version of ref.<sup>/33/</sup> is adopted. Only quadrupole deformations are permitted. The values of the corresponding deformation parameter  $\epsilon$  are the experimental ones taken from the compilations  $^{/34,35/}$ . If no experimental values for  $\epsilon$  are given the deformation is estimated extrapolating linearly within a chain of isotones. The values used are indicated in fig. 2. In the expressions (2.10), (3.3) the contributions from matrix-elements between different oscillator shells ( $\Delta N=\pm 2$ ) are taken into account.

The strength of the pairing interaction G is parametrized with the help of the averaged-gap-method proposed in ref/<sup>34/</sup>. The averaged gap  $\tilde{\Delta}$  determines G via the averaged level density  $\tilde{\rho}$ . It is convenient to approximate  $\tilde{\rho}$  ba means of the asymptotic expression given in ref.<sup>(35/</sup>):

 $\tilde{\tilde{\rho}}_{Z,N}(x) = h \omega_0^{-1} \left[ \left( \frac{x}{h \omega_0} \right)^2 - \frac{1}{4} \left( 1 + \frac{2}{9} \epsilon^2 \right) + \alpha_{Z,N} \left( \frac{x}{h \omega_0} \right)^4 \right], \quad (5.1)$ 

where  $h\omega_0$  is the oscillator constant of the Nilsson-model. The values  $a_Z = 2.33 \cdot 10^{-3} + 0.108\epsilon^2$  and  $a_N = 1.19 \cdot 10^{-3} + 0.008\epsilon^2$  are obtained from a comparison of expression (5.4) with the values of the averaged level density calculated directly from the Nilssonmodel by means of the Strutinsky-averagingprocedure \*.

The averaged gap is determined from the values of the expressions  $P_Z, P_N$ (see ref.<sup>36/</sup> expr. (2.92), (2.93);  $P_Z, P_N$  are denoted there by  $\Delta_P, \Delta_n$  calculated from the experimental binding energies of 4 adjacent nuclides.

\* The author is indebted to Dr. V.V.Pashkevich for kindly supplying the computer code.

In the rare earth region the  $P_Z$  and  $P_N$ -values within a chain of isotopes decrease with increasing mass number A (see fig. 1). In order to take into account this effect a Z, N -dependence of the averaged gap is introduced

$$\widetilde{\tilde{\Lambda}}_{Z,N} = \frac{\Lambda}{A^{\frac{1}{2}}} \{1 - \eta \left[ \left( \frac{\Delta v(Z,N)}{v_{Z=N}} \right)^2 - \left( \frac{\Delta v(\overline{Z},\overline{N})}{v_{Z=N}} \right)^2 \right] \}, (5.2)$$

where

$$\frac{\Delta v(Z, N)}{v_{Z=N}} = \left(\frac{2Z, 2N}{A}\right)^{1/3} - 1, \ \overline{Z}, \overline{N} = \frac{A \mp 0.4A^2}{A + 200}.$$



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Fig. 1. The pairing gap and the P-values for the rare earth region. The experimental binding energies are taken from ref.<sup>45/</sup>. The values of ref.<sup>46/</sup> are preferred if larger accuracy is indicated. The number of strings indicates how many values of the binding energy in the expression for P correspond to extrapolations of nuclear masses (see ref.<sup>45/</sup>). In the first part of the figure  $\Lambda_0 = 13.9$  MeV whereas in the second part  $\Lambda_0 = 13.1$  MeV is chosen.

In these expressions  $v_{Z=N}$  means the velocity of particles at the Fermi-surface in the case, N = Z. Av is the deviation from this value for given Z or N<sup>/36</sup>, Z,N are the numbers of nucleons on the line of  $\beta$ -stability<sup>/37</sup>. The idea behind the expressions (5.2) is that the strength of pair-correlations should be related to  $v^{/33}$ . An expression de-

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pending only linearly on  $\Delta v/v_{Z=N}$  fails to reproduce the fact that both  $P_Z$  and  $P_N$  decrease with increasing mass number. Thus, a quadratic dependence has been assumed. The correction term  $(\Delta v(\overline{Z},\overline{N})/v_{Z=N})^2$  is subtracted because the Z,N -dependence of  $\overline{\Delta}$  corresponding to the line of  $\beta$ -stability is already incorporated in the leading term  $\Delta_0/\Lambda^2$ .

Comparing directly the calculated and experimental values of  $P_N$  and  $P_7$  we found the parameters  $\eta = 120$  and, respectively,  $\Delta_0 = 13.9$  MeV and  $\Delta_0 = 13.1$  MeV for the beginning and the end of the rare earth region. The theoretical values of  $P_{\gamma}$  and  $P_{N}$ are obtained from the ground state energies  $E_0$  calculated with the deformation  $\epsilon$  corresponding to the nuclid Z,N.The expression for the ground state energy of odd nuclei can be easily obtained from the expression for the "two-quasiparticle energy" (A7) by removing the second blocked level ; The values of  $\Delta_0$  found for the rare earth region agree reasonably well with the value of 12 MeV /34, 36/ for the whole periodic table. The calculated and experimental values of  $P_{\chi}$ ,  $P_{N}$  are shown in fig. 1. It is interesting to compare the calculations with and without Q-projection. The most striking feature is the increase of the gap  $\Delta$  if the particle number is conserved. This effect leads to an increase of the difference between P and  $\Delta$  because the Pvalues are not very much influences by Q projection. Therefore it is not correct to determine the pairing strength by comparing the experimental values of P directly with  $\Delta$ , as usually done in BCS-approximation.

Rather, one must relate the experimental and theoretical values of P. The values of the parameters obtained in this way are also suitable for the BCS-approximation.

## 5. <u>Discussion of the Region of Low</u> Angular Momentum

The results of the calculations are presented in fig. 2 as graphs of the moment of inertia as a function of the square of the angular velocity  $\omega$ . Only Q-projection is taken into account. The discussion of  $P_{I}$  -projection is postponed to section 7. The points of the function  $f(\omega^2)$  are obtained in the following (direct) way: For given the angular velocity  $\omega$  equals to I/4where  $\int equals$  to expr. (2.10) taken at the minimum of  $E_I$  with respect to  $\Delta_Z$  and  $\Delta_N$ . In order to determine the function  $\mathfrak{I}(\omega^2)$ from the experimental spacing of the yrast levels the exprs. (13) and (14d) in ref.  $^{/3/}$ are used. The example in fig. 3 demonstrates that the points of  $\mathfrak{g}(\omega^2)$  obtained by means of this method from the calculated values of  $E_1$  agree rather well with those obtained in the direct way. In the case of less pronounced bb. the agreement is still better.

Let us first consider the region of low angular velocity where  $\mathfrak{g}$  approximately linearly depends on  $\omega^2$ . The comparison of theoretical and experimental results in this region permits one to get an impression to what extend the predictions for high angular momenta can be trusted. It can be seen in fig. 2 that the calculated moments of iner-



tia at I = 0 are smaller than the experimental ones. In BCS-approximation the average deviation amounts to 25%. If Q-projection is taken into account it increases by 10%. This discrepancy has been known for a long time  $^{/38/}$ . As a calculation with



Fig. 3. The inclination  $dJ/d\omega^2$  of the linnear part of  $J(\omega^2)$  for the nuclei of the rare earth region. The contribution of CAP is calculated in the present work. The contributions from the change of the quadrupole and hexadecapole deformation as well as the 4th order cranking correction are taken, respectively, from tabs. V and VI of ref.<sup>23/</sup>.

reduced pairing strength shows (see section 7) it is too large to be connected wit the uncertainties the strength of pairing is determined with. In refs. /26,31/ corrections to expression (2.11) are proposed which allow one to reproduce the experimental moments of inertia with good accuracy. In the present work we do not further consider the very interesting problem of the theoretical prediction of the moment of inertia. Rather we concentrate on nonadiabatic effects assuming that the missing contribution to the moment of inertia does not depend on angular momentum. As is easil seen a constant correction to the moment of inertia leads only to a corresponding constant shift of all points of  $\int (\omega^2)$  along the  $\mathfrak{I}$ -axis. The shape of the curve remains unchanged. Therefore we simply compare the shifted curves. Some aspects of the possibility that the correction to the moment of inertia depends on angular momentum are discussed in section 7.

The inclination of the linear part of the theoretical curves  $\int (\omega^2)$  is mainly determined by the stiffness of the system with respect to a change of  $\Delta$ . It can be seen in figs. 2 and 4 that the inclination of the curves with account of Q-projection is always lower than that of the curves corresponding to the BCS-approximation. This larger stability of pairing is connected with the fact that particle number conservation increases the pair-correlation energy by approximately a factor of 2 and this leads to a larger curvature of the function  $E_0(\Delta)$  at the equilibrium point.



The calculated value of the inclination  $d q/d \omega^2$  is smaller than in experiment. This does not mean any failure of the Q-projection method, but merely expresses the fact that there are important nonadiabatic effects besides CAP. In fig. 4 the contributions arising from the singleparticle degrees of freedom ("4th order cranking contribution"), guadrupole and hexadecapole deformation are added to the value of  $d \frac{4}{d\omega^2}$ obtained in the present work for the CAP. It is shown in ref. /22/that in the linear region the contributions from different nonadiabatic effects simply add. The numbers corresponding to the mentioned nonadiabatic effects are taken from ref.  $^{/24/}$  (The quantity  $C_{VIM}^{-1}$  calculated there equals to  $2d \frac{q}{d\omega^2}$  ). After taking into account the additional effects the inclination of the linear part of  $\mathfrak{g}(\omega^2)$ is reproduced with good accuracy for the stable deformed nuclei. The agreement between calculated and experimental values is somewhat better than in ref. /36/, presumably because the Q.projection is carried out exactly. It should be mentioned the main contribution to  $d \frac{g}{d\omega^2}$ comes from the single-particle degrees of freedom.

The good agreement of the theoretical and experimental values for the inclination in the case of well deformed nuclei is interpreted as an indication that CAP is quantitatively correct described by the Q-projected BCS-function.

If the contribution of CAP to the total value of  $dg/d\omega^2$  is calculated in BCS-approximation, the inclination is obtained larger than experimentally observed. In this approximation the sole CAP gives already the experimental value. This coincidence has often been used  $^{/8,9,17-21/}$  as an argument in favour of a description of nonadiabatic effects in terms of only the CAP and the change of deformation.

For the nuclei at the borders of the deformed region the theoretical value of the inclination with Q-projection is smaller than the experimental one. This indica tes a limination of the method of ref.<sup>/18/</sup>. Most likely the deformation degrees of freedom are not properly dealt with.

#### 6. The Critical Angular Velocity

In order to discuss the region of high angular momentum in a guantitative way it is useful to define a critical angular velocity  $\omega_{cr}$ , where the transition from the suprafluid to the normal state takes place. The quantity  $\omega_{cr}$  is introduced by means of a simplified version of the analysis of bb in terms of crossing bands as suggested in refs.  $^{/16,39/}$ . It is assumed that the transition can be described by the crossing of a paired band with the moment of inertia  $\mathfrak{f}_1$  corresponding to the ground state, and an unpaired band with the moment of inertia 4, which equals to the value after the break-down of pairing. The unpaired band begins at  $\delta E_0 = E_0(\Delta(1=0)) + E_0(\Delta = 0)$ , i.e., at the total pair correlation energy in the ground state. A constant interaction V between the bands is assumed. Then the energy of the yrast line reads

$$E_{I} = \frac{1}{2} \left[ \delta E_{0} + \frac{\hat{I}^{2}}{2g_{1}} + \frac{\hat{I}^{2}}{2g_{2}} - \sqrt{\left( \delta E_{0} + \frac{\hat{I}^{2}}{2g_{2}} - \frac{\hat{I}^{2}}{2g_{1}} \right)^{2} + 4V^{2}} \right] \cdot (6.1)$$

Following refs.  $^{/37,38/}$  the phase transition is is characterized by the branch out

$$(\delta E_0 + \frac{e_{cr}^2}{2q_1} - \frac{e_{cr}^2}{2q_2}) + 4V^2 = 0$$
 (6.2)

in the complex  $e^2$ -plane. The critical angular momentum  $I^2_{cr}$ , where the transition takes place is defined as the real part of  $e^2_{cr}$ 

 $\hat{I}_{cr}^{2} = \frac{2\delta E_{0}}{g_{2} - g_{1}}g_{1}g_{2}.$  (6.3)

The imaginary part of  $e_{cr}^2$  determines the degree of abruptness of the transition, which is not important for the discussion to be followed. The moment of inertia at the transition point equals the value

$$\mathcal{G}_{cr} = \frac{1}{2} \left( \frac{dE}{dI} \right)^{-1}_{I=I_{cr}} = \frac{1}{2} \left( \mathcal{G}_{1} + \mathcal{G}_{2} \right) \frac{\mathcal{G}_{1} \mathcal{G}_{2}}{\frac{1}{4} \left( \mathcal{G}_{1} + \mathcal{G}_{2} \right)^{2}} \approx 0.8 \frac{\mathcal{G}_{1} + \mathcal{G}_{2}}{2}.(6.4)$$

where for the ratio of the geometric and arithmetic means a typical value for the rare earth region is taken. The critical angular velocity is given by

moment of inertia in the ground state). In

this way one can reduce the uncertainties due to the fact that expr. (6.1) which is appropriate for the very transition region does not give a good description of the linear part of  $\mathfrak{f}(\omega^2)$ . If  $\mathfrak{f}(\omega^2)$  shows a pronounced bb, it is better to determine  $\omega_{\rm cr}$ from the approximate relation

$$\omega_{\rm cr} = \frac{1}{2} (\omega_1 + \omega_2) , \qquad (6.6)$$

where  $\omega_{\frac{1}{2}}$  are the turning points of the S-shaped function  $\mathfrak{f}(\omega^2)$ . Eq. (6.6) can easily be obtained considering that  $\omega_{\frac{1}{2}}$ approximately equals to  $I_{cr}/\mathfrak{f}_{\frac{1}{2}}$  is the ratio  $V/\delta E_0$  is small (pronounced bb).

The critical angular velocity is displayed in fig. 5. An estimate of the possible errors shows that the uncertainty of  $\omega_{cr}^2$ is less than ±0.01 MeV<sup>2</sup> in the case of a steep increase of  $\mathfrak{f}(\omega^2)$  around  $\hat{\mathbf{I}}_{cr}$  whereas it may increase up to ±0.03 MeV<sup>2</sup> in the case of a very smooth behaviour of  $\mathfrak{f}(\omega^2)$ . This is a sufficient accuracy for the discussion of bb in the next section.

#### 7. Discussion of the Transition Region

It is shown in fig. 5 that the square of the critical angular velocity at which the proton pairing vanishes lies between 0.2 and 0.3 MeV<sup>2</sup>. The systematic decrease of  $\omega_{cr}^2$  within a chain of isotopes is a consequence of the proposed dependence of the pairing strength on Z and N.The irregularities in the isotopes of  $E_r$  and Yb are connected with fluctuations of the level density due to the crossing of levels.

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with no cul G -projection MeV denotes the critical  $\Delta_0 = 12$  MeV C and  $\Delta_0$ strength guare of t
The line pairing e i uclo ā reduced earth Fig

. For almost all nuclei the neutron-pairing vanishes at a smaller angular velocity than the proton-pairing. The value of  $\omega_{cr}^2$ equals about 0.12 MeV  $^2$  in the whole rare earth region. The dips of  $\omega_{cr}^2$  at N = 98 and N = 102, 104 are connected with local minima of the level density (see also ref. /8/ ). The break-down of neutronpairing is accompanied by bb for most of the nuclei for which the effect is observed experimentally (see fig. 2). However the value of  $\omega_{cr}^2$  which corresponds to the functions  $f(\omega^2)$  obtained from the experimental spacings of the yrast levels equals about  $0.07 \text{ MeV}^2$  in the whole rare earth region. Hence, bb is observed at a systematically lower angular velocity than the value at which the break-down of pairing is predicted.

This result possesses a serious problem for the interpretation of bb in terms of CAP. We shall even go one step further suggesting that the angular velocity at which bb is observed is not large enough to cause the transition to the nonsuprafluid state. This means that CAP should not be responsible for bb. As this important conclusion is based on the magnitude of  $\omega_{cr}^2$  it is necessary to consider the relevance of the calculated values in more detail.

As was already discussed in section 5, the BCS-approximation leads to a lower stability of the suprafluid state than Q-projection, reflected by the correspondingly low value of  $\omega_{\rm cr}^2 = 0.07 \, {\rm MeV}^2$ . This is illustrated by typical numbers obtained for the rare earth region:  $\delta E_0 = 2.2 \, {\rm MeV}$  with Q-projection,  $\delta E_0 = 1.5 \, {\rm MeV}$  without and  $f_2 - f_1 =$ 

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= 40 MeV<sup>-1</sup> in both cases. From (6.5) one obtains the estimates  $\omega_{cr}^2 = 0.13$  MeV<sup>2</sup> and  $\omega_{cr}^2 = 0.09$  MeV respectively, which are somewhat higher than those in fig. 5. The difference equals 0.04 MeV<sup>2</sup> close to the value in fig. 5. The larger pair correlation energy in the number conserving approach is obvious: Q-projection corresponds to an improvement of the wave function of the paired band and therefore, leads to a decrease of the energy. The unpaired band remaines unchanged by Q-projection.

We have investigated the stability of  $\omega^2$ with respect to a variation of the parameter of the pairing strength. A reduction of  $\Delta_0$  to 12 MeV yields a value of  $\omega_{cr}^2 =$ = 0.11 MeV<sup>2</sup> (see fig. 5). The quantities  $P_Z$ and  $P_N$  are reduced by about the same amount as  $\Delta_0$ . Although there are some uncertainties as to what extend effects other than pairing do inefluence the P-values, it seems that the uncertainties in determining the pairing strength should not be much larger than the investigated variation of  $\Delta_0$ . A reduction of the pairing strength which is strong enough to push  $\omega_{cr}^2$  down to the value at which bb is observed would be incompatible with the experimental values of  $P_Z$  and  $P_N$ . Similarly the discrepancy between the calculated and experimental values of  $\mathfrak{g}(\omega^2)$  at  $\omega = 0$  cannot be explained by the uncertainties of the pairing strength because the investigated reduction of  $\Delta_0$ increases  $\mathfrak{f}(0)$  only by 10%.

The curvature of the function  $E_0(\Delta_0)$  at its minimum and the depth  $\delta E_0$  of the minimum are closely related. The inclination of the linear part of  $\mathfrak{f}(\omega^2)$  is proportional to the curvature<sup>/18/</sup>. As was discussed in the previous section the experimental value of this quantity is reproduced with a good accuracy. This can be considered as an independent indication that our calculations provide a good estimate of  $\delta E_0$ .

As was mentioned in sect. 5, the moment of inertia in the ground state  $g_1$  is obtained smaller than observed. However, the typical value  $g_2 = 60 \text{ MeV}^{-1}$  for the moment of inertia after the gbreak-down of neutron-pairing seems to be of the right order because it corresponds to the rigid body moment for the neutrons. If for  $g_1$ the typical experimental value of 30 MeV<sup>-1</sup> is taken and  $\delta E_0$  is kept equal tp 2.2 MeV the critical velocity increases to  $\omega_{cr}^2 =$ = 0.17 MeV<sup>2</sup>.

It is possible to avoid the uncertainties in the calculation of the moment of inertia by taking the experimental value of  $\mathfrak{f}_{\mathfrak{g}} - \mathfrak{f}_{\mathfrak{g}}$ from the S-shaped curves. Use of the typical experimental values  $\mathfrak{f}_{9}-\mathfrak{f}_{1}=40$  MeV<sup>-1</sup> and  $\omega_{cr}^2 = 0.07 \text{ MeV}^2$  (6.5) permits one to calculate an "experimental" energy  $\delta E_0 = 1.5 \text{ MeV}^2$ where the second band begins. (This value is close to those of refs. /37,38/ obtained from a more sophisticated phenomenological analysis). The energy of the head of the band causing bb is significantly smaller than the pair correlation energy for which 2.2 MeV is a typical value. Thus also from this point of view it is obvious that the unpaired band lies too high to permit a crossing with the paired band at that value of the angular momentum where bb is observed. a start start of a star

Let us now consider the consequences of the conservation of angular momentum. As was discussed in section 3 the P<sub>I</sub>-projection influence the CAP via the correction to the ground state energy (see expr. (3.1)) and corrections to the rotational energy which are of higher order in I<sup>2</sup>. The correction to  $E_0$  leads to an increase of  $\Delta$  for given G. In contrast to the Q-projection the quantities  $P_Z$  and  $P_N$  calculated with the correction (3.1) show approximately the same increase as A. (The dispersion of angular momentum is almost the same for odd and even nuclei). This increase of  $P_7$  and  $P_N$  must be compensated by a reduction of the pairing strength. The value  $\Delta_0 = 11.5$  MeV reproduces in good approximation the  $P_N$  values without corrections of the ground state energy. The strength of proton pairing is slightly overestimated. As can be seen from the example in fig. 3, the curves with and without the correction to the ground state energy almost coincide. The same result has been obtained for other nuclei not presented in fig. 3. In order to investigate the role of the terms of higher order in  $I^2$  fig. 3 shows a comparison the functions  $\mathfrak{J}(\omega^2)$  calculated from expr. (3.4) and from the ground state energy (3.1) plus  $1^2/2 \oint_{PY}$ (i.e., the quadratic approximation of expr. (3.4)). It is demonstrated that the higher order terms do not significantly change the value of  $\omega_{cr}^2$ . The same result has been found in more systematic calculations/40,41/. From the discussion of the  $P_{\rm I}$  projection it is concluded that the conservation of angular momentum does not lead to any essential change of  $\omega_{cr}^2$ .

The above discussions have provided a certain confidence in value of the critical frequency of the break-down of neutron-pairing. Now the conclusion from the beginning of this section is emphasized: For the nuclei of the rare earth region the angular velocity at which bb is observed is not enough to cause a transition of the neutron system into the nonsuprafluid state. Therefore the present quantitative analysis does not confirm the interpretation of bb in terms of CAP. (The same statement is made in ref.<sup>/15/</sup>).

As is already extensively discussed the value of  $\omega_{cr}^2$  becomes considerably larger if the conservation of particle number is taken into account, because the total pair-correlation energy is substantially increased. In the case of RAL similar changes are not expected because the two-quasiparticle energies and the relevant matrix-elements are not very sensitive to Q-projection. This fact is reflected by the calculated moments of inertia.

RAL is also essential for the interpretation of the following result of calculations: In the case of nuclei with  $90 \le N \le 94$  the moment of inertia after the breakdown of neutron-pairing is larger than both the experimental and the rigid body value. Inspecting the individual contribution of each two-quasiparticle state to expr. (2.10) it turns out that the large value is due to the terms from the states with K = 1/2 and 3/2 discending from the  $i_{13/2}$ ; subshell. It is quite obvious that the contributions from these levels cannot be treated by perturbation theory.

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They tend to decouple from the core keeping the moment of inertia small /7/.

From the point of view of the alternative explanations of bb mentioned in the introduction the negative conclusion concerning the CAP means a confirmation of the interpretation in terms of RAL. Howeve: was as discussed in refs.  $^{/12,13,15/}$  CAP and RAL are only two aspects of the more complex phenomenon of the phase transition from the suprafluid to the normal state in a rotating nucleus. The transition does no take place for the whole system at once, rather the pair correlations vanish first for levels with high angular momentum. The angular velocity at which this occurs for the  $i_{1,3/2}$  neutron level, is estimated  $\frac{15}{3}$ to be just that where bb is observed. As the neutrons on the depaired levels are le stable bound to the rotating core they ten to align their angular momenta to the axis of rotation. At higher angular velocity the pair correlations vanish also for the levels with smaller angular momentum until the nucleus is in the nonsuprafluid state.

With regard to this picture the critica angular velocity calculated in thos work represents the upper limit for the existen of pairing in the rotating nucleus. Although the results are obtained by means of perturbation theory, they are also relevant in the case of strong RAL. This can be seen from the following argument: It is shown in ref.  $^{/42/}$  that near the ground state equilibrium deformation the value of the moment of inertia obtained by perturba tion theory approximately equals to an ave raged value from which the influences of

shell structure are eliminated. Furthermore it is shown, that the value of the averaged rotational energy is only very weakly influenced by nonadiabatic effects arising from the single-particle degrees of freedom (for details see ref. /42/ 3). Therefore, the critical angular velocity can be understood as the limit for the existence of pairing if shell structure is not included in the rotational energy. Shell structure may cause a partial depairing of levels with high angular momentum ( $i_{13/2}$  neutron-levels) at  $\omega < \omega_{cr}$ . Since the contributions of single-particle degrees of freedom to the inclination of  $f(\omega^2)$ at  $\omega = 0$  are larger than expected for the averaged rotational energy, shell structure only promotes the depairing of certain levels. Hence, the critical angular velocity plotted on fig. 5 really represents an upper limit for the existence of pairing in the rotating nucleus. For nuclei with N = 94 this interpretation is not quite correct because the obtained moment of inertia after break-down of pairing is larger than expected for the averaged behaviour (see fig. 2).

The investigations of CAP in refs.  $^{/8,43/}$ yield a considerably smaller value of  $\omega_{cr}^2$ than that obtained in the present work. In refs.  $^{/7,45/}$  the rotational energy is calculated by means of the simple P<sub>I</sub>-projection (see section 3). As was already discussed, P<sub>I</sub> -projection does not essential influence CAP. The difference  $f_2-f_1$  obtained in refs.  $^{/7,45/}$ is indeed not far from our value. Therefore, the smaller value of  $\omega_{cr}^2$  must be connected with a corresponding smaller value of

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the pair correlation energy  $\delta E_0$ . The smaller value of  $\delta E_0$  is a consequence of the fact that in ref.<sup>/8/</sup> only 2 meshpoints are taken in order to approximate the O-projection integral (A8) (In the present work 8 meshpoints are used). In ref.  $^{/43/}$  the number of mesh-points is increased to 4, but at the same time the pairing strength is reduced keeping  $\Delta$  constant. As was already discussed above such a reduction which keeps  $\omega_{cr}^2$  approximately at value of  $0.07 \text{ MeV}^2$  is not compatible with the experimental value of  $P_N$ . Furthermore the small value of  $\delta E_0$  corresponds to an inclination of the linear part of  $\mathfrak{g}(\omega^2)$  which is significantly larger than the experimental value if, as necessary, the contributions from the single-particle degrees of freedom are added (see section 5).

#### 8. Conclusions

A systematic investigation of the CAP has been carried out for the nuclei of the rare earth region. For the parametrization of the pairing strength a new two-parameterexpression is suggested which reproduces the even-odd mass differences with a good accuracy. As already noticed in a number of previous investigations it turned out in the calculations that using a realistic strength of (monopole) pairing the moment of inertia in the ground state is obtained smaller than observed. Although there are several suggestions explaining the discrepancy it seems that the problem needs to be finally clarified. 

Considering only the CAP the inclination of the linear part of the moment of inertia as function of the square of the angular velocity is obtained smaller than observed. However, if the contributions from all expected nonadiabatic effects are taken into account a very good agreement of the theoretical and experimental values of the inclination is found in the case of stable deformed nuclei. The most important contribution comes from the single particle degrees of freedom. As the present calculations provide a good description of nonadiabatic effects in the spectrum at low angular momentum they should also yield reliable predictions concerning the CAP at high angular momentum.

The calculations show that the exact conservation of angular momentum does not significantly influence the CAP. However, the exact conservation of particle number turned out to be very essential for a quantitative description of CAP. In comparison with the BCS-approximation the number conserving approach yields a considerably higher value of the total pair-correlation energy which is decisive for the stiffness of the system with respect to a change of strength of the pair-correlations.

In the rare earth region the calculations predict the neutron pairing to breakdown at the square of the angular velocity of about 0.12 MeV<sup>2</sup>. Although there exists a correlation between the numbers of nucleons for which bb really appears and those for which a rapid transition accompanied by bb is theoretically predicted, the sudden increase of the moment of inertia causing

bb is observed at a square of the angular velocity of about 0.07 MeV<sup>2</sup> noticeably smaller than the angular velocity of the break.down of pairing. From this it is concluded that the exprementally observed bb does not correspond to a break-down of neutron pairing. The angular frequency at which bb is observed is not high enough to destroy all pair correlations. Bb should rather be connected with the depairing of few levels with high angular momentum ( $i_{13/2}$ neutron levels in rare earth region) and a simultaneous alignment of the collective and corresponding particle angular momenta. This mechanism represents the first step of the transition from the suprafluid to th normal state in the rotating nucleus.

Analogous to the critical field in a superconductor the critical angular velocity calculated in this work is interpreted as the upper limit for the existence of the suprafluide phase. Conservation of particle number leads to a considerable increase of the critical angular velocity in comparison with estimates based on the BSCapproximation. In the rare earth region the neutron pairing is predicted to vanish at a value of angular momentum of about 24h whe reas the proton pairing is predicted to vanish between 40h and 60h.

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#### Appendix

For the evaluation of the matrix-elements one needs the commutation relations

$$Q_{N}c_{i}^{+} = c_{i}^{+}Q_{N-1}, \quad Q_{N}c_{i} = c_{i}Q_{N+1}$$

and the relations describing the action of  $\epsilon^+_i$  and  $\mathbf{c}_i$  on the BCS-function

$$c_{i}^{+}|\Delta,\lambda\rangle = c_{i}^{+}u_{i}|\Delta,\lambda,i\rangle, c_{i}|\Delta,\lambda\rangle = c_{i}^{+}v_{i}|\Delta,\lambda,i\rangle,$$

$$c_{i}^{+}|\Delta,\lambda\rangle = c^{+}u_{i}|\Delta,\lambda,i\rangle, c_{i}|\Delta,\lambda\rangle = -c_{i}^{+}v_{i}|\Delta,\lambda,i\rangle,$$
(A1)

where i > 0 and  $|\Delta, \lambda, i>$  denotes that the level i is blocked, i.e., left out in the product (2.4). All expressions are reduced to the normalization integrals

 $\mathfrak{N}_{0} = <\Delta, \lambda | Q_{N} | \Delta, \lambda >, \ \mathfrak{N}_{i} = <\Delta, \lambda, i | Q_{N-1} | \Delta, \lambda, i >, \ \mathfrak{N}_{ij} = <\Delta, \lambda, ij | Q_{N-2} | \Delta, \lambda, ij >,$ 

where  $<\Delta,\lambda,ij>$ means a BCS-function with the levels i,j blocked. The expectation value of H is given by

$$<\Delta, N | H_{sp} | \Delta, N > = \Re_{0}^{-1} <\Delta, \lambda | Q_{N} \sum_{i} \epsilon_{i} c_{i}^{+} c_{i} | \Delta, \lambda >,$$
  
$$<\Delta, N | H_{sp} | \Delta, N > = 2 \sum_{i>} \epsilon_{i} v_{i}^{2} \frac{\Re_{i}}{\Re_{0}},$$
 (A2)

and

$$\langle \Delta, N | P^{\dagger}P | \Delta, N \rangle = \mathfrak{N}_{0}^{-1} \langle \Delta, \lambda | Q \underset{\substack{N \\ i \geq -i \geq }}{\Sigma} c_{i}^{\dagger}c_{i}^{\dagger}c_{j}^{\dagger} | \Delta, \lambda \rangle,$$

$$<\Delta, N | P^{\dagger}P | \Delta, N > = \Re_{0}^{-1} \sum_{v_i v_j} <\Delta, \lambda, i | Q_{N-2} | \Delta, \lambda, j >,$$
 (A3)

$$\langle \Delta, \mathbf{N} | \mathbf{P}^{\dagger} \mathbf{P} | \Delta, \mathbf{N} \rangle = \sum_{i \geq \neq j \geq v_{i} \mathbf{v}_{i} \mathbf{v}_{j} \mathbf{v}_{j} \frac{\mathcal{N}_{ij}}{\mathcal{N}_{0}} + \sum_{i \geq v_{i}^{2}} \mathbf{v}_{i}^{2} \frac{\mathcal{N}_{ij}}{\mathcal{N}_{0}} ,$$

$$\langle \Delta, \mathbf{N} | \mathbf{P}^{\dagger} \mathbf{P} | \Delta, \mathbf{N} \rangle = \sum_{i \geq i, j \geq v_{i} \geq v_{i} \mathbf{v}_{j} \mathbf{v}_{j} \frac{\mathcal{N}_{ij}}{\mathcal{N}_{0}} - \sum_{i \geq v_{i}^{2}} \mathbf{v}_{i}^{4} \frac{\mathcal{N}_{ij}}{\mathcal{N}_{0}} .$$

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The last sum represents a renormalization of the single-particle levels due to the pairing interaction. As usual, this term is neglected.

Orthogonality of the states  $|\Delta, N, ij\rangle$ can be easily seen from the expression  $\langle \Delta, N, ij | \Delta, N, i'j \rangle = (\Re_{ij} \Re_{i'j})^{-\frac{1}{2}} \langle \Delta, \lambda, ij | c_j c_i c_i^+ c_j^+ Q_{N-2} | \Delta, \lambda, i'j\rangle$ Carrying out some commutations one obtains  $\langle \Delta, N, ij | \Delta, N, i'j \rangle = (\Re_{ij} \Re_{i'j})^{-\frac{1}{2}} \langle \Delta, \lambda, ij | c_i^+ c_j c_i c_j^+ Q_{N-2} | \Delta, \lambda, i'j\rangle$  $+ \delta_{ii'} [\delta_{jj'} - (\Re_{ij} \Re_{i'j})^{-\frac{1}{2}} \langle \Delta, \lambda, ij | c_j^+ c_j Q_{N-2} | \Delta, \lambda, i'j \rangle] - (A4)$  $-\delta_{ji'} [\delta_{ij'} - (\Re_{ij} \Re_{i'j})^{-\frac{1}{2}} \langle \Delta, \lambda, ij | c_j^+ c_j Q_{N-2} | \Delta, \lambda, i'j \rangle].$ 

From eq. (A1) follows that the creation operator applied on the blocked BCS-function on the left hand side either gives zero or is changed into a annihilation operator of the time reversed state. As only the case  $i \neq j$  is considered this operator commutes with all other ones and gives zero acting on the blocked BCS-function on the right-hand side. Thus, orthonormality is shown. Following the same arguments it is obvious that  $\langle \Delta, N, ij | \Delta, N \rangle = 0$  if  $i \neq j$ 

As  $H_{sp}$  is a diagonal single-operator it can be shown in the same manner as for the states that nondiagonal matrix-elements vanish. The diagonal term reads

 $<\!\!\Delta, N, ij \mid \!H_{sp} \mid \!\Delta, N, ij \!\!> = \epsilon_i + \epsilon_j + \Re_{ij}^{-1} <\!\!\Delta, \lambda, ij \mid \!H_{sp} \!Q_{N-2} \mid \!\Delta, \lambda, ij \!\!> \!\!(A5)$ 

In the case of the pairing interaction new terms arise from the commutator  $[P, c_i^{\dagger}] = c_{\tilde{i}}$ . However, the operator  $c_{\tilde{i}}$  gives zero acting on the blocked BCS-function on the righthand side. The same argument is valid for  $P^+$ and the BCS-function on the left-hand side. The diagonal term reads

 $\langle \Delta, N, ij | P^{+}P | \Delta, N, ij \rangle = \Re_{ij}^{-1} \langle \Delta, \lambda, ij | P^{+}PQ_{N-2} | \Delta, \lambda, ij \rangle. (A6)$ 

Hence the "two-quasiparticle energy" equals

$$E_{ij} = \epsilon_i + \epsilon_j + E_0^{ij} (N-2) , \qquad (A7)$$

where  $E_0^{ij}(N-2)$  means the ground state energy of a system of N-2 particles with the levels i,j blocked. The corresponding expression can be easily obtained from eqs. (A2) and (A3) if the levels ij are removed from the sums and the normalization integrals. Applying eq. (A1) to the matrix-element  $\langle \Delta, N, ij | J_x | \Delta. N \rangle = (\Re_{ij} \Re_0)^{-\frac{1}{2}} \langle \Lambda, \lambda, ij | Q_{N-2} c_j c_{ij} c_{j} c_{j$ 

one gets

 $<\Delta, N, ij \mid J \mid \Lambda, N > = (\mathcal{N}_{ij} \mathcal{N}_0)^{-1/2} \times$ 

 $\times \sum_{i > j >} u_i w_j <\Delta, \lambda, ij | C_{N-2} c_j c_i (j_{i'j}^{x} c_i^+ c_i^+ - j_i^{x} - c_i^+ c_j^+) | \Delta, \lambda, i'j > .$ 

From the orthogonality of the states  $|\Lambda,N,ij\rangle$  follows

$$\langle \Lambda, N, ij | J_x | \Lambda, N \rangle = -\left(\frac{\mathcal{H}_{ij}}{\mathcal{H}_0}\right)^{\frac{1}{2}} \left(u_i v_j - u_j v_i\right) j_{ij}^x$$
, (A8)

where the convention  $-i = i \cdot i = 0$  is used. As  $J_x$  generates from  $(\Lambda, N)$  only the states  $[\Lambda, N, ij]$  and [I] is diagonal within this set, one gets

 $\langle \Delta, N | J_{\mathbf{x}} \begin{pmatrix} \mathbf{H} \\ 1 \end{pmatrix} J_{\mathbf{x}} | \Delta, N \rangle = \frac{1}{2} \sum_{ij} | \Delta, N, ij | J_{\mathbf{x}} | \Delta, N \rangle |^{2} \begin{pmatrix} \mathbf{E}_{ij} \\ 1 \end{pmatrix} . (A8)$ 

By means of eqs. (A7) and (A8) one immediately obtains expr. (3.3).

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In order to evaluate the normalization integrals the integral representation  $^{/44/}$  of  $Q_N$  is applied:

 $Q_{N} = \frac{1}{2\pi} \int_{0}^{2\pi} d\phi e^{i\phi(N-N)}$ , where N denotes the operator of particle number. A straight-forward calculation, provides

 $\mathfrak{N}_{0} = \frac{1}{2\pi} \int_{0}^{2\pi} d\phi e^{i\phi N} \prod_{i>} (u_{i}^{2} + v_{i}^{2} e^{-2i\phi}).$ (A8)

The form of the other normalization integra is obvious. In the calculations the integra is approximated by a ifinite sum over equidistant mesh-points.

As is shown in ref.<sup>/44/</sup>  $2^{\nu}$  mesh-points ensure that all admixtures corresponding to N  $\pm \Delta N$ ,  $0 < \Delta N < 2^{\nu+1}$  are eliminated. In practical calculations  $\nu = 3$  turned out to be sufficient. A further increase of  $\nu$  does not lead to any significant change of the results.

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